total power of the formulas was used. Owing to the fact that the probability distribution for the normalized structure factor E is always approximately

$$\frac{1}{\sqrt{2\pi}} \exp\left(-\tfrac{1}{2}E^2\right),$$

all structures are equally vulnerable to the attack by probability methods.

In view of these considerations, we looked forward, with the appearance of the Monograph, to a period of cooperation with crystallographers interested in applying the method, since the very essence of the scientific method consists in the direct confrontation of a plausible theory with an experimental problem. Indeed, we have recently enjoyed the privilege of cooperating with Christ, Clark & Evans (1954) in their study of the structure of colemanite, and the successful application of these methods is described in the note which follows.

In view of the successful solution of the colemanite structure, the appearance of the previous two notes is unfortunate since they tend to discourage further applications of method.

With regard to the note of Cochran & Woolfson (1954), there is no logical basis for their interpretation of the validity of our formulas in terms of the Patterson function. Furthermore, while they implicitly admit the existence of a bias in the separate terms of Σ_4, they conclude that this bias can never be revealed, no matter how many terms Σ_4 may contain. This conclusion contradicts well known laws of probability and is in disagreement with column 5 of Table 14 in the Monograph.

The note of Vand & Pepinsky (1954) is vague and logically disconnected. Their claim that our formulas are approximate is misleading because, as implied on the top of p. 39 of the Monograph, any desired accuracy can be obtained by using a sufficient number of terms in the series expansion of (3·03). Naturally we listed only those terms which in our experience appeared to be required. In any event, it is difficult to understand how more accurate general distributions can be obtained from empirical tables.

Their claim that our formulas are related to the Patterson function in the way they describe has not been justified and, in view of the theoretical derivation and the experimental verification of our formulas, their claim *cannot* be justified. Also, it is not at all clear how individual formulas admittedly having the correct bias can lead to incorrect answers when a sufficient number of structure factors are used jointly.

For $P\bar{1}$, it is true that Σ_1 contains only one term, and consequently is unimportant as a phase-determining formula for this space group. For the other space groups, however, Σ_1 contains several terms and is an important phase-determining relation. Thus Σ_1 is included in the formulas for $P\bar{1}$ merely for completeness; the term Σ_4, which may contain hundreds of terms, is much more important. The terms Σ_2 and Σ_3 are also very important in the intermediate stages of the phase-determining procedure. It is therefore difficult to understand why these terms have been omitted from their consideration while the unimportant Σ_1 occupies a central position in their note. Furthermore, it should be noted that in $P\bar{1}$, Σ_1 and Σ_4 apply only to those structure factors whose indices h, k, l are all even.

The general impression given by the note of Vand & Pepinsky is that our solution of the phase problem 'does not represent anything of greater power than that of previously known methods' (e.g. the use of Harker maps), whereas they claim to have discovered new formulas of greater power. Their example of such a formula is the coefficient of $U_{2h,0,2l}$ in their last equation. They apparently failed to realize that this is *identical* with our equation (4·41) on p. 63 of the Monograph and has been used by us to help determine the signs of $E_{2h,0,2l}$ for naphthalene. (Note that they refer to $P2_1/c$ instead of our $P2_1/a$.)

In conclusion we would welcome further opportunities to cooperate with other crystallographers in applying these methods to the study of structures in the various centrosymmetric space groups.

References

CHRIST, C. L., CLARK, J. R. & EVANS, H. T., JR. (1954). *Acta Cryst.* 7, 453.

COCHRAN, W. & WOOLFSON, M. M. (1954). *Acta Cryst.* 7, 450.

HAUPTMAN, H. & KARLE, J. (1953). *Solution of the Phase Problem. I. The Centrosymmetric Crystal.* ACA Monograph No. 3. Wilmington: The Letter Shop.

VAND, V. & PEPINSKY, R. (1954). *Acta Cryst.* 7, 451.

Acta Cryst. (1954). 7, 453

The structure of colemanite, $CaB_3O_4(OH)_3.H_2O$, determined by the direct method of Hauptman & Karle.*

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The present note describes the preliminary structure of colemanite, $CaB_3O_4(OH)_3.H_2O$, obtained through the use of the direct method of crystal-structure determination given by Hauptman & Karle (1953).

In order to compute the E^2_{hkl}'s required by the method, 3084 F^2_{hkl}'s (including 1056 non-observed F^2_{hkl}'s), obtained by visual estimation, were used to determine the $K(s)$ curve (Karle & Hauptman, 1953). Using all 3084 E^2_{hkl}'s the signs of the 2028 non-zero F_{hkl}'s were calculated. For 183 (9%) of these non-zero terms the sign was indeterminate. However, only the sums Σ_1, Σ_2, and Σ_3 were used in the sign determinations, and only a small percentage of the total available number of contributors to each of these sums was used. It seems clear from this that at least most of the remaining 183 signs could have been obtained using the full power of the method had it been necessary for this preliminary investigation.

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The major portion of these calculations was made using IBM facilities. However, it was found that after certain preliminary computations, it would have been feasible to have found the signs (at the rate of about 100–150 per day) without the use of automatic computing machinery. The detailed procedures for the calculations of the signs were worked out by Karle, Hauptman & Christ and will be published separately at a later date.

For the preliminary structure analysis 944 observed F_{hkl}'s, together with their signs, were used to calculate electron-density sections over the xz plane at intervals of 1/60 for $y = 0$ to $y = 1/4$. The 944 terms used are those contained within a sphere of radius equal to $\sin\theta/\lambda = 0{\cdot}66$ Å^{-1}. In order to minimize termination-of-series effects, an artificial temperature factor $\exp[-B(\sin\theta/\lambda)^2]$, with $B = 2{\cdot}5$ Å^2, was multiplied into the observed F_{hkl}'s.

Colemanite is monoclinic $P2_1/a$,

$$a = 8{\cdot}743 \pm 0{\cdot}004,\quad b = 11{\cdot}264 \pm 0{\cdot}002,\quad c = 6{\cdot}102 \pm 0{\cdot}003 \text{ Å},\quad \beta = 110°\ 7',$$

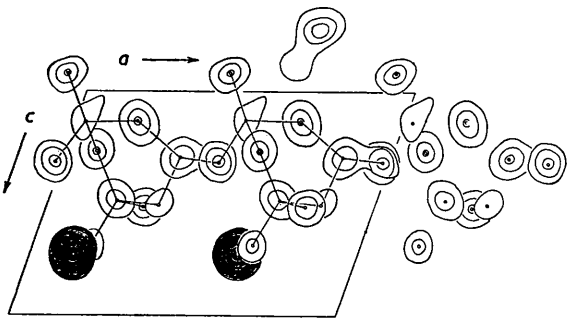

Fig. 1. Composite projection on (010) of the electron-density sections for colemanite. Only a portion sufficient to show the essential features of the structure is given. The small black circles indicate the boron positions, the small open circles the oxygen positions.

$Z = 4$; the calculated density is 2·419 g.cm.$^{-3}$, the observed density 2·42 g.cm.$^{-3}$ (Christ, 1953).

A composite projection on (010) of the electron-density sections is shown in Fig. 1. This shows clearly that there are infinite boron–oxygen chains running parallel to the a axis, the chain element being made up of a BO_3 triangle and two BO_4 tetrahedra forming a ring. The chain element has the composition $[B_3O_4(OH)_3]^{-2}$. Each Ca^{++} is roughly octahedrally coordinated by 5 oxygens and 1 water molecule. The formula for colemanite may thus be written $CaB_3O_4(OH)_3.H_2O$. The average B–O bond length in the tetrahedra is $1{\cdot}4_3$ Å, and in the triangles is $1{\cdot}3_7$ Å. Ca^{++} has as nearest neighbors 5 oxygens and 1 water molecule at an average distance of $2{\cdot}4_4$ Å. The discrepancy factor R for the $hk0$ zone is 25%.

This work was made possible only through the wholehearted cooperation of a number of people. G. J. Mowitt and Mrs Violet Rice made available the facilities of the U.S. Geological Survey IBM Section; Vincent Latorre of this Section was mainly responsible for the calculation of the electron-density sections. Mr Peter O'Hara of the Computation Laboratory of the National Bureau of Standards carried out most of the IBM calculations of the signs. As mentioned above, Drs Karle and Hauptman of the Naval Research Laboratory worked intensively with one of us (C.L.C) on the procedures for sign calculations. We are greatly indebted to all of these persons.

References

CHRIST, C. L. (1953). *Amer. Min.* **38**, 411.
HAUPTMAN, H. & KARLE, J. (1953). *Solution of the Phase Problem. I. The Centrosymmetric Crystal.* ACA Monograph No. 3. Wilmington: The Letter Shop.
KARLE, J. & HAUPTMAN, H. (1953). *Acta Cryst.* **6**, 473.

Acta Cryst. (1954). **7**, 454

Divisors for converting $\sin^2\theta$ for a standard wavelength.*

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In determining precision lattice parameters by X-ray diffraction (e.g. Cohen's method) it is common to use the $\sin^2\theta$ form of the Bragg equation. It then becomes convenient to convert values of $\sin^2\theta$ for several wavelengths to a value representing one standard wavelength for the purpose of calculation. We have found that a table listing divisors for converting $\sin^2\theta(\lambda')$ to $\sin^2\theta(\lambda)$, where λ is a desired standard wavelength, is very helpful in speeding computations by calculating machine. Such a table is based on the wavelengths in Ångström units (Table 1) given by Lonsdale (1950), although of course the divisors apply also to calculations based on kX. units. Conversion divisors for these wavelengths, the ratio $(\lambda'/\lambda)^2$, are listed in Table 2, and also, for convenience, the values of $\lambda^2/3$ and $\lambda^2/4$.

Table 1. *Wavelengths of emission lines of certain elements*

Element	$K\alpha_1$	$K\alpha_2$	$K\beta_1$
Cr	2·28962 Å	2·29351 Å	2·08480 Å
Mn	2·10175	2·10569	1·91015
Fe	1·93597	1·93991	1·75653
Co	1·78892	1·79278	1·62075
Ni	1·65784	1·66169	1·50010
Cu	1·54051	1·54433	1·39217
Zn	1·43511	1·43894	1·29522
Ga	1·34003	1·34394	1·20784
Ge	1·25401	1·25797	1·12890
Mo	0·70926	0·71354	0·63225
Ag	0·55936	0·56378	0·49701

Reference

LONSDALE, K. (1950). *Acta Cryst.* **3**, 400.

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